Lecture 9: Support Vector Machines Advanced Topics in Machine Learning: COMPGI13

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- The representer theorem
- Review of convex optimization
- \bullet Support vector classification, the C-SV and $\nu\text{-}\text{SV}$ machines

Representer theorem

Given a set of paired observations $(x_1, y_1), \ldots, (x_n, y_n)$ (regression or classification). Find the function f^* in the RKHS \mathcal{H} which satisfies

$$f^* = \arg\min_{f \in \mathcal{H}} J(f), \tag{1}$$

where

$$J(f) = L_y(f(x_1), \ldots, f(x_n)) + \Omega\left(\|f\|_{\mathcal{H}}^2 \right),$$

 Ω is non-decreasing, y is the vector of y_i , loss L depends on x_i only via $f(x_i)$.

- Classification: $L_y(f(x_1), \ldots, f(x_n)) = \sum_{i=1}^n \mathbb{I}_{y_i f(x_i) \le 0}$
- Regression: $L_y(f(x_1), ..., f(x_n)) = \sum_{i=1}^n (y_i f(x_i))^2$

The representer theorem: a solution to

$$\min_{f\in\mathcal{H}}\left[L_{y}(f(x_{1}),\ldots,f(x_{n}))+\Omega\left(\left\|f\right\|_{\mathcal{H}}^{2}\right)\right]$$

takes the form

$$f^* = \sum_{i=1}^n \alpha_i k(x_i, \cdot).$$

If Ω is strictly increasing, the solution must have this form.

Proof: Denote f_s projection of f onto the subspace

$$\operatorname{span}\left\{k(x_i,\cdot):\ 1\leq i\leq n\right\},\tag{2}$$

such that

$$f=f_s+f_{\perp},$$

where $f_s = \sum_{i=1}^{n} \alpha_i k(x_i, \cdot)$. Regularizer:

$$\|f\|_{\mathcal{H}}^2 = \|f_s\|_{\mathcal{H}}^2 + \|f_{\perp}\|_{\mathcal{H}}^2 \ge \|f_s\|_{\mathcal{H}}^2,$$

then

$$\Omega\left(\|f\|_{\mathcal{H}}^{2}\right) \geq \Omega\left(\|f_{s}\|_{\mathcal{H}}^{2}\right),$$

so this term is minimized for $f = f_s$.

Proof (cont.): Individual terms $f(x_i)$ in the loss:

$$f(x_i) = \langle f, k(x_i, \cdot) \rangle_{\mathcal{H}} = \langle f_s + f_{\perp}, k(x_i, \cdot) \rangle_{\mathcal{H}} = \langle f_s, k(x_i, \cdot) \rangle_{\mathcal{H}},$$

SO

$$L_y(f(x_1),\ldots,f(x_n))=L_y(f_s(x_1),\ldots,f_s(x_n)).$$

Hence

- Loss *L*(...) only depends on the component of *f* in the data subspace,
- Regularizer $\Omega(\ldots)$ minimized when $f = f_s$.
- If Ω is non-decreasing, then $\|f_{\perp}\|_{\mathcal{H}} = 0$ is a minimum. If Ω strictly increasing, min. is unique.

Short overview of convex optimization

Why we need optimization: SVM idea

Classify two clouds of points, where there exists a hyperplane which linearly separates one cloud from the other without error.



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Why we need optimization: SVM idea

Classify two clouds of points, where there exists a hyperplane which linearly separates one cloud from the other without error.



Smallest distance from each class to the separating hyperplane $w^{\top}x + b$ is called the margin.

This problem can be expressed as follows:

$$\max_{w,b} (\operatorname{margin}) = \max_{w,b} \left(\frac{2}{\|w\|} \right) \quad \text{or} \quad \min_{w,b} \|w\|^2 \tag{3}$$

subject to

$$\begin{cases} (w^{\top}x_i + b) \ge 1 & i : y_i = +1, \\ (w^{\top}x_i + b) \le -1 & i : y_i = -1. \end{cases}$$
(4)

This is a convex optimization problem.



(Figure from Boyd and Vandenberghe)

Leftmost set is convex, remaining two are not.

Every point in the set can be seen from any other point in the set, along a straight line that never leaves the set.

Definition

C is convex if for all $x_1, x_2 \in C$ and any $0 \leq \theta \leq 1$ we have $\theta x_1 + (1 - \theta)x_2 \in C$, i.e. every point on the line between x_1 and x_2 lies in *C*.

Convex function: no local optima



(Figure from Boyd and Vandenberghe)

Definition (Convex function)

A function f is convex if its domain domf is a convex set and if $\forall x, y \in \text{dom} f$, and any $0 \le \theta \le 1$,

$$f(\theta x + (1 - \theta)y) \le \theta f(x) + (1 - \theta)f(y).$$

The function is **strictly convex** if the inequality is strict for $x \neq y$.

Optimization and the Lagrangian

(Generic) optimization problem on $x \in \mathbb{R}^n$,

minimize
$$f_0(x)$$

subject to $f_i(x) \le 0$ $i = 1, ..., m$ (5)
 $h_i(x) = 0$ $i = 1, ..., p.$

• p^* the optimal value of (5), \mathcal{D} assumed nonempty, where...

• $\mathcal{D} := \bigcap_{i=0}^{m} \operatorname{dom} f_{i} \cap \bigcap_{i=1}^{p} \operatorname{dom} h_{i}$ (dom f_i =subset of \mathbb{R}^{n} where f_i defined).

Ideally we would want an unconstrained problem

minimize
$$f_0(x) + \sum_{i=1}^m I_-(f_i(x)) + \sum_{i=1}^p I_0(h_i(x))$$
,

where
$$I_{-}(u) = \begin{cases} 0 & u \leq 0 \\ \infty & u > 0 \end{cases}$$

Why is this hard to solve?

and $I_0(u)$ is the indicator of 0.

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D := ∩_{i=0}^m dom f_i ∩ ∩_{i=1}^p dom h_i (dom f_i =subset of ℝⁿ where f_i defined).
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Lower bound interpretation of Lagrangian

The Lagrangian $L : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$ is a lower bound on the original problem:

$$L(x,\lambda,\nu) := f_0(x) + \sum_{i=1}^m \underbrace{\lambda_i f_i(x)}_{\leq I_-(f_i(x))} + \sum_{i=1}^p \underbrace{\nu_i h_i(x)}_{\leq I_0(h_i(x))},$$

and has domain dom $L := \mathcal{D} \times \mathbb{R}^m \times \mathbb{R}^p$. The vectors λ and ν are called lagrange multipliers or dual variables. To ensure a lower bound, we require $\lambda \succeq 0$.



The Lagrange dual function: minimize Lagrangian When $\lambda \succeq 0$ and $f_i(x) \le 0$, Lagrange dual function is

$$g(\lambda,\nu) := \inf_{x \in \mathcal{D}} L(x,\lambda,\nu).$$
(6)

A dual feasible pair (λ, ν) is a pair for which $\lambda \succeq 0$ and $(\lambda, \nu) \in \text{dom}(g)$. We will show: (next slide) for any $\lambda \succeq 0$ and ν ,

 $g(\lambda,\nu) \leq f_0(x)$

wherever

$$\begin{array}{ll} f_i(x) & \leq 0 \\ h_i(x) & = 0 \end{array}$$

(including at $f_0(x^*) = p^*$).

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(including at $f_0(x^*) = p^*$).

Simplest example: minimize over x the function $L(x, \lambda) = f_0(x) + \lambda f_1(x)$ (Figure modified from Boyd and Vandenberghe)



Reminders:

- f₀ is function to be minimized.
- f₁ ≤ 0 is inequality constraint
- $\lambda \ge 0$ is Lagrange multiplier
- *p*^{*} is minimum *f*₀ *in constraint set*

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When $\lambda \succeq 0$, then for all ν we have

$$g(\lambda,\nu) \le p^* \tag{7}$$

A dual feasible pair (λ, ν) is a pair for which $\lambda \succeq 0$ and $(\lambda, \nu) \in \operatorname{dom}(g)$ (Figure from Boyd and Vandenberghe)





- $\lambda \ge 0$ is Lagrange multiplier
- p* is minimum f₀ in constraint set

Lagrange dual is lower bound on p^* (proof)

We now give a formal proof that Lagrange dual function $g(\lambda, \nu)$ lower bounds p^* .

Proof: Assume \tilde{x} is feasible, i.e. $f_i(\tilde{x}) \leq 0$, $h_i(\tilde{x}) = 0$, $\tilde{x} \in D$, $\lambda \succeq 0$. Then

$$\sum_{i=1}^m \lambda_i f_i(\tilde{x}) + \sum_{i=1}^p \nu_i h_i(\tilde{x}) \le 0$$

Thus

$$g(\lambda,\nu) := \inf_{x\in\mathcal{D}} \left(f_0(x) + \sum_{i=1}^m \lambda_i f_i(x) + \sum_{i=1}^p \nu_i h_i(x) \right)$$

$$\leq f_0(\tilde{x}) + \sum_{i=1}^m \lambda_i f_i(\tilde{x}) + \sum_{i=1}^p \nu_i h_i(\tilde{x})$$

$$\leq f_0(\tilde{x}).$$

This holds for every feasible \tilde{x} , hence lower bound holds.

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Best lower bound $g(\lambda, \nu)$ on the optimal solution p^* of (5): Lagrange dual problem

maximize
$$g(\lambda, \nu)$$

subject to $\lambda \succeq 0.$ (8)

Dual feasible: (λ, ν) with $\lambda \succeq 0$ and $g(\lambda, \nu) > -\infty$. Dual optimal: solutions (λ^*, ν^*) maximizing dual, d^* is optimal value (dual always easy to maximize: next slide). Weak duality always holds:

$$d^* \leq p^*$$
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...but what is the point of finding a **best (largest) lower bound** on a **minimization problem**?

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Best lower bound: maximize the dual

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Dual feasible: (λ, ν) with $\lambda \succeq 0$ and $g(\lambda, \nu) > -\infty$. Dual optimal: solutions (λ^*, ν^*) to the dual problem, d^* is optimal value (dual always easy to maximize: next slide). Weak duality always holds:

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Strong duality: (does not always hold, conditions given later):

$$d^* = p^*$$

If S.D. holds: solve the easy (concave) dual problem to find p^* .

Maximizing the dual is always easy

The Lagrange dual function: minimize Lagrangian (lower bound)

$$g(\lambda,\nu) = \inf_{x\in\mathcal{D}} L(x,\lambda,\nu).$$

Dual function is a pointwise infimum of affine functions of (λ, ν) , hence concave in (λ, ν) with convex constraint set $\lambda \succeq 0$.



Example:

One inequality constraint,

$$L(x,\lambda) = f_0(x) + \lambda f_1(x),$$

and assume there are only four possible values for x. Each line represents a different x.

How do we know if strong duality holds?

Conditions under which strong duality holds are called **constraint qualifications** (they are sufficient, but not necessary)

(Probably) best known sufficient condition: Strong duality holds if

• Primal problem is **convex**, i.e. of the form

minimize $f_0(x)$ subject to $f_i(x) \le 0$ i = 1, ..., n (10) Ax = b $(h_i \text{ affine})$

for convex f_0, \ldots, f_m , and

 Slater's condition holds: there exists some strictly feasible point¹ x̃ ∈ relint(D) such that

$$f_i(\tilde{x}) < 0$$
 $i = 1, \ldots, m$ $A\tilde{x} = b.$

¹We denote by $\operatorname{relint}(\mathcal{D})$ the relative interior of the set \mathcal{D} . This looks like the interior of the set, but is non-empty even when the set is a subspace of a larger space.

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for convex f_0, \ldots, f_m , and

• **Slater's condition** for the case of **affine** f_i is trivial (inequality constraints no longer strict, reduces to original inequality constraints)

$$f_i(\tilde{x}) \leq 0$$
 $i = 1, \ldots, m$ $A\tilde{x} = b$.

A consequence of strong duality...

Assume primal is equal to the dual. What are the consequences?

- *x*^{*} solution of original problem (minimum of *f*₀ *under constraints*),
- (λ^*, ν^*) solutions to dual

$$f_{0}(x^{*}) = g(\lambda^{*}, \nu^{*})$$

$$= \inf_{\substack{(\text{assumed})}} \left(f_{0}(x) + \sum_{i=1}^{m} \lambda_{i}^{*} f_{i}(x) + \sum_{i=1}^{p} \nu_{i}^{*} h_{i}(x) \right)$$

$$\leq \inf_{\substack{(\text{inf definition})}} f_{0}(x^{*}) + \sum_{i=1}^{m} \lambda_{i}^{*} f_{i}(x^{*}) + \sum_{i=1}^{p} \nu_{i}^{*} h_{i}(x^{*})$$

$$\leq f_{0}(x^{*}),$$

(4): (x^*, λ^*, ν^*) satisfies $\lambda^* \succeq 0$, $f_i(x^*) \le 0$, and $h_i(x^*) = 0$.

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Assume primal is equal to the dual. What are the consequences?

- x* solution of original problem (minimum of f₀ under constraints),
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$$\begin{array}{ll} f_0(x^*) & = & g(\lambda^*, \nu^*) \\ & = & \inf_{\substack{(\text{assumed})}} & \int_{x \in \mathcal{D}} \left(f_0(x) + \sum_{i=1}^m \lambda_i^* f_i(x) + \sum_{i=1}^p \nu_i^* h_i(x) \right) \\ & \leq & \\ & (\text{inf definition}) & f_0(x^*) + \sum_{i=1}^m \lambda_i^* f_i(x^*) + \sum_{i=1}^p \nu_i^* h_i(x^*) \\ & \leq & \\ & \leq & \\ & (4) & f_0(x^*), \end{array}$$

(4): (x^*, λ^*, ν^*) satisfies $\lambda^* \succeq 0$, $f_i(x^*) \le 0$, and $h_i(x^*) = 0$.

From previous slide,

$$\sum_{i=1}^{m} \lambda_i^* f_i(x^*) = 0, \tag{11}$$

which is the condition of complementary slackness. This means

$$egin{array}{lll} \lambda_i^* > 0 & \Longrightarrow & f_i(x^*) = 0, \ f_i(x^*) < 0 & \Longrightarrow & \lambda_i^* = 0. \end{array}$$

From λ_i , read off which inequality constraints are strict.
KKT conditions for global optimum

Assume functions f_i , h_i are differentiable and strong duality. Since x^* minimizes $L(x, \lambda^*, \nu^*)$, derivative at x^* is zero,

$$abla f_0(x^*) + \sum_{i=1}^m \lambda_i^* \nabla f_i(x^*) + \sum_{i=1}^p \nu_i^* \nabla h_i(x^*) = 0.$$

KKT conditions definition: we are at **global optimum**, $(x, \lambda, \nu) = (x^*, \lambda^*, \nu^*)$ when (a) **strong duality** holds, and (b)

primal feasibility

dual feasibility complementary slackness $\begin{array}{rcl} f_i(x) & \leq & 0, \ i = 1, \dots, m \\ h_i(x) & = & 0, \ i = 1, \dots, p \\ \lambda_i & \geq & 0, \ i = 1, \dots, m \\ \lambda_i f_i(x) & = & 0, \ i = 1, \dots, m \end{array}$

zero derivatives

$$\nabla f_0(x) + \sum_{i=1}^m \lambda_i \nabla f_i(x) + \sum_{i=1}^p \nu_i \nabla h_i(x) = 0$$

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zero derivatives
$$\nabla f_0(x) + \sum dx$$

$$\nabla f_0(x) + \sum_{i=1}^m \lambda_i \nabla f_i(x) + \sum_{i=1}^p \nu_i \nabla h_i(x) = 0$$

In summary: if

- primal problem convex and
- constraint functions satisfy Slater's conditions

then strong duality holds. If in addition

• functions f_i , h_i differentiable

then KKT conditions necessary and sufficient for optimality.

Linearly separable points

Classify two clouds of points, where there exists a hyperplane which linearly separates one cloud from the other without error.



Smallest distance from each class to the separating hyperplane $w^{\top}x + b$ is called the margin.

Maximum margin classifier, linearly separable case

This problem can be expressed as follows:

$$\max_{w,b} (\operatorname{margin}) = \max_{w,b} \left(\frac{2}{\|w\|} \right)$$
(12)

subject to

$$\begin{cases} \min(w^{\top}x_{i}+b) = 1 & i : y_{i} = +1, \\ \max(w^{\top}x_{i}+b) = -1 & i : y_{i} = -1. \end{cases}$$
(13)

The resulting classifier is

$$y = \operatorname{sign}(w^{\top}x + b),$$

We can rewrite to obtain

$$\max_{w,b} \frac{1}{\|w\|} \quad \text{or} \quad \min_{w,b} \|w\|^2$$

subject to

$$y_i(w^{\top}x_i+b)\geq 1.$$

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subject to

$$y_i(w^{\top}x_i+b) \geq 1.$$
 (14)

Maximum margin classifier: with errors allowed

Allow "errors": points within the margin, or even on the wrong side of the decision boundary. Ideally:

$$\min_{w,b}\left(\frac{1}{2}\|w\|^2+C\sum_{i=1}^n\mathbb{I}[y_i\left(w^{\top}x_i+b\right)<0]\right),$$

where *C* controls the tradeoff between maximum margin and loss. Replace with convex, continuous upper bound:

$$\min_{w,b} \left(\frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \theta \left(y_i \left(w^\top x_i + b \right) \right) \right)$$

with hinge loss,

$$\theta(\alpha) = (1 - \alpha)_{+} = \begin{cases} 1 - \alpha & 1 - \alpha > 0\\ 0 & \text{otherwise.} \end{cases}$$

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Substituting in the hinge loss, we get

$$\min_{w,b} \left(\frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \theta \left(y_i \left(w^\top x_i + b \right) \right) \right).$$

How do you implement hinge loss with simple inequality constraints (for optimization)?

$$\min_{w,b,\xi} \left(\frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i \right)$$
(15)

subject to²

$$\xi_i \ge 0$$
 $y_i\left(w^{\top}x_i+b\right) \ge 1-\xi_i$

²Either $y_i(w^{\top}x_i + b) \ge 1$ and $\xi_i = 0$ as before, or $y_i(w^{\top}x_i + b) < 1$, and then $\xi_i > 0$ takes the value satisfying $y_i(w^{\top}x_i + b) = 1 - \xi_i$.

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$$\xi_i \geq 0$$
 $y_i\left(w^{\top}x_i+b\right) \geq 1-\xi_i$

²Either $y_i(w^{\top}x_i + b) \ge 1$ and $\xi_i = 0$ as before, or $y_i(w^{\top}x_i + b) < 1$, and then $\xi_i > 0$ takes the value satisfying $y_i(w^{\top}x_i + b) = 1 - \xi_i$.



Does strong duality hold?

Is the optimization problem convex wrt the variables w, b, ξ ?

$$\begin{array}{ll} \text{minimize} & f_0(w, b, \xi) := \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i \\ \text{subject to} & f_i(w, b, \xi) := 1 - \xi_i - y_i \left(w^\top x_i + b \right) \leq 0 \quad i \in 1, \dots, n \\ & f_j(w, b, \xi) := -\xi_j \leq 0 \qquad \qquad j \in 1, \dots, n \end{array}$$

Each of f_0, f_1, \ldots, f_n are convex.

② Does Slater's condition hold? Trivial since inequality constraints affine, and there always exists some

$$\begin{aligned} \xi_i &\geq 0\\ y_i \left(w^\top x_i + b \right) &\geq 1 - \xi_i \end{aligned}$$

Thus **strong duality** holds, the problem is differentiable, hence the KKT conditions hold at the global optimum.

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The Lagrangian: $L(w, b, \xi, \alpha, \lambda)$

$$= \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i + \sum_{i=1}^n \alpha_i \left(1 - y_i \left(w^\top x_i + b \right) - \xi_i \right) + \sum_{i=1}^n \lambda_i (-\xi_i)$$

with dual variable constraints

$$\alpha_i \geq 0, \qquad \lambda_i \geq 0.$$

Minimize wrt the primal variables w, b, and ξ .

Support vector classification: Lagrangian

Derivative wrt w:

$$\frac{\partial L}{\partial w} = w - \sum_{i=1}^{n} \alpha_i y_i x_i = 0 \qquad w = \sum_{i=1}^{n} \alpha_i y_i x_i.$$
(16)

Derivative wrt b:

$$\frac{\partial L}{\partial b} = \sum_{i} y_{i} \alpha_{i} = 0.$$
(17)

Derivative wrt ξ_i :

$$\frac{\partial L}{\partial \xi_i} = C - \alpha_i - \lambda_i = 0 \qquad \alpha_i = C - \lambda_i.$$
(18)

Noting that $\lambda_i \geq 0$,

$$\alpha_i \leq C.$$

Now use complementary slackness:

Non-margin SVs: $\alpha_i = C \neq 0$:

- We immediately have $1 \xi_i = y_i (w^\top x_i + b)$.
- ② Also, from condition α_i = C λ_i, we have λ_i = 0 (hence can have ξ_i > 0).
- Margin SVs: $0 < \alpha_i < C$:
 - We again have $1 \xi_i = y_i \left(w^\top x_i + b \right)$

② This time, from $\alpha_i = C - \lambda_i$, we have $\lambda_i \neq 0$, hence $\xi_i = 0$. Non-SVs: $\alpha_i = 0$

- 1 This time we can have: $y_i (w^\top x_i + b) > 1 \xi_i$
- **2** From $\alpha_i = C \lambda_i$, we have $\lambda_i \neq 0$, hence $\xi_i = 0$.

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- This time we can have: $y_i (w^{\top} x_i + b) > 1 \xi_i$
- 2 From $\alpha_i = C \lambda_i$, we have $\lambda_i \neq 0$, hence $\xi_i = 0$.

We observe:

- The solution is sparse: points which are not on the margin, or "margin errors", have $\alpha_i = 0$
- The support vectors: only those points on the decision boundary, or which are margin errors, contribute.
- Influence of the non-margin SVs is bounded, since their weight cannot exceed C.

Support vector classification: dual function

Thus, our goal is to maximize the dual,

$$g(\alpha, \lambda) = \frac{1}{2} \|w\|^{2} + C \sum_{i=1}^{n} \xi_{i} + \sum_{i=1}^{n} \alpha_{i} \left(1 - y_{i} \left(w^{\top} x_{i} + b\right) - \xi_{i}\right) \\ + \sum_{i=1}^{n} \lambda_{i} (-\xi_{i}) \\ = \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j} + C \sum_{i=1}^{m} \xi_{i} - \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j} \\ - b \sum_{i=1}^{m} \alpha_{i} y_{i} + \sum_{i=1}^{m} \alpha_{i} - \sum_{i=1}^{m} \alpha_{i} \xi_{i} - \sum_{i=1}^{m} (C - \alpha_{i}) \xi_{i} \\ = \sum_{i=1}^{m} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j}.$$

Support vector classification: dual function

Maximize the dual,

$$g(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j x_i^{\top} x_j,$$

subject to the constraints

$$0 \leq \alpha_i \leq C, \quad \sum_{i=1}^n y_i \alpha_i = 0$$

This is a quadratic program.

Offset *b*: for the margin SVs, we have $1 = y_i (w^{\top} x_i + b)$. Obtain *b* from any of these, or take an average.

Support vector classification: kernel version



Taken from Schoelkopf and Smola (2002)

Maximum margin classifier in RKHS: write the hinge loss formulation

$$\min_{w} \left(\frac{1}{2} \|w\|_{\mathcal{H}}^{2} + C \sum_{i=1}^{n} \theta\left(y_{i} \left\langle w, k(x_{i}, \cdot) \right\rangle_{\mathcal{H}} \right) \right)$$

for the RKHS \mathcal{H} with kernel $k(x, \cdot)$. Use the result of the representer theorem,

$$w(\cdot) = \sum_{i=1}^n \beta_i k(x_i, \cdot).$$

Maximizing the margin equivalent to minimizing $||w||_{\mathcal{H}}^2$: for many RKHSs a smoothness constraint (e.g. Gaussian kernel).

Support vector classification: kernel version

Substituting and introducing the ξ_i variables, get

$$\min_{\beta,\xi} \left(\frac{1}{2} \beta^{\top} K \beta + C \sum_{i=1}^{n} \xi_i \right)$$
(19)

where the matrix K has i, jth entry $K_{ij} = k(x_i, x_j)$, subject to

$$\xi_i \geq 0$$
 $y_i \sum_{j=1}^n \beta_j k(x_i, x_j) \geq 1 - \xi_i$

Convex in β , ξ since K is positive definite: hence strong duality holds.

Dual:

$$g(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j k(x_i, x_j),$$

subject to $w(\cdot) = \sum_{i=1}^{n} y_i \alpha_i k(x, \cdot), \quad 0 \le \alpha_i \le C.$

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subject to $w(\cdot) = \sum_{i=1}^{n} y_i \alpha_i k(x, \cdot), \quad 0 \le \alpha_i \le C.$

Another kind of SVM: the ν -SVM:

Hard to interpret C. Modify the formulation to get a more intuitive parameter ν .

Again, we drop b for simplicity. Solve

$$\min_{w,\rho,\xi} \left(\frac{1}{2} \|w\|^2 - \nu\rho + \frac{1}{n} \sum_{i=1}^n \xi_i \right)$$

subject to

$$\begin{array}{rrr} \rho & \geq & 0 \\ \xi_i & \geq & 0 \\ y_i w^\top x_i & \geq & \rho - \xi_i, \end{array}$$

(now directly adjust margin width ρ).

The ν -SVM: Lagrangian

$$\frac{1}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^n \xi_i - \nu \rho + \sum_{i=1}^n \alpha_i \left(\rho - y_i w^\top x_i - \xi_i \right) + \sum_{i=1}^n \beta_i (-\xi_i) + \gamma (-\rho)$$

for dual variables $\alpha_i \geq 0$, $\beta_i \geq 0$, and $\gamma \geq 0$.

Differentiating and setting to zero for each of the primal variables w, ξ , ρ ,

$$w = \sum_{i=1}^{n} \alpha_i y_i x_i$$

$$\alpha_i + \beta_i = \frac{1}{n}$$

$$\nu = \sum_{i=1}^{n} \alpha_i - \gamma$$
(20)

From $\beta_i \ge 0$, equation (20) implies $0 \le \alpha_i \le n^{-1}$. From $\gamma \ge 0$ and (21), we get $\nu \le \sum_{i=1}^n \alpha_i$.

$$\frac{1}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^n \xi_i - \nu \rho + \sum_{i=1}^n \alpha_i \left(\rho - y_i w^\top x_i - \xi_i \right) + \sum_{i=1}^n \beta_i (-\xi_i) + \gamma (-\rho)$$

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Complementary slackness conditions:

Assume $\rho >$ 0 at the global solution, hence $\gamma =$ 0, and

$$\sum_{i=1}^{n} \alpha_i = \nu. \tag{22}$$

Case of $\xi_i > 0$: complementary slackness states $\beta_i = 0$, hence from (20) we have $\alpha_i = n^{-1}$. Denote this set as $N(\alpha)$. Then

$$\sum_{i\in N(\alpha)}\frac{1}{n}=\sum_{i\in N(\alpha)}\alpha_i\leq \sum_{i=1}^n\alpha_i=\nu,$$

SO

$$\frac{|N(\alpha)|}{n} \le \nu,$$

and ν is an upper bound on the number of non-margin SVs.

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and ν is an upper bound on the number of non-margin SVs.

Case of $\xi_i = 0$: $\beta_i > 0$ and so $\alpha_i < n^{-1}$. Denote by $M(\alpha)$ the set of points $n^{-1} > \alpha_i > 0$. Then from (22),

$$\nu = \sum_{i=1}^{n} \alpha_i = \sum_{i \in \mathcal{N}(\alpha)} \frac{1}{n} + \sum_{i \in \mathcal{M}(\alpha)} \alpha_i \le \sum_{i \in \mathcal{M}(\alpha) \cup \mathcal{N}(\alpha)} \frac{1}{n}$$

thus

$$u \leq \frac{|N(\alpha)| + |M(\alpha)|}{n},$$

and ν is a lower bound on the number of support vectors with non-zero weight (both on the margin, and "margin errors").

Dual for ν -SVM

Substituting into the Lagrangian, we get

$$\frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha_{i}\alpha_{j}y_{i}y_{j}x_{i}^{\top}x_{j} + \frac{1}{n}\sum_{i=1}^{n}\xi_{i} - \rho\nu - \sum_{i=1}^{m}\sum_{j=1}^{m}\alpha_{i}\alpha_{j}y_{i}y_{j}x_{i}^{\top}x_{j}$$
$$+ \sum_{i=1}^{n}\alpha_{i}\rho - \sum_{i=1}^{n}\alpha_{i}\xi_{i} - \sum_{i=1}^{n}\left(\frac{1}{n} - \alpha_{i}\right)\xi_{i} - \rho\left(\sum_{i=1}^{n}\alpha_{i} - \nu\right)$$
$$= -\frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha_{i}\alpha_{j}y_{i}y_{j}x_{i}^{\top}x_{j}$$

Maximize:

$$g(\alpha) = -\frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j x_i^{\top} x_j,$$

subject to

$$\sum_{i=1}^n \alpha_i \ge \nu \qquad 0 \le \alpha_i \le \frac{1}{n}.$$
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